

Theory of ultrafast processes in molecules

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I will give a tutorial lecture about the theoretical description of ultrafast dynamics in molecules. I will first discuss the circumstances under which electron and nuclear dynamics are coupled. I will then present an overview of the ab initio theoretical chemistry methods able to model such coupled electron-nuclear dynamics (Figure 1) [1, 2]. Finally, I will present case studies from my own work, illustrating several of these methods and simulating various molecular processes induced by light [3, 4, 5, 6].

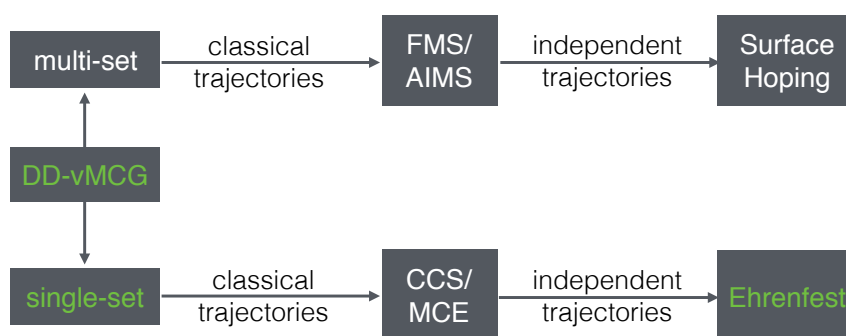


Figure 1: Schematic representation of the relationships among ab initio methods, able to describe non-adiabatic dynamics [1].

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